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Illinois Quantum Information Science and Technology Center

Machine Learning for Quantum Computing and Quantum Matter

Bryan Clark

Department of Physics - University of Illinois at Urbana Champaign

Center for Artificial Intelligence Innovation; October 5, 2020

Machine Learning Quantum Matter and Quantum Computing

Majoranas in superconductors

arXiv:2008.09128

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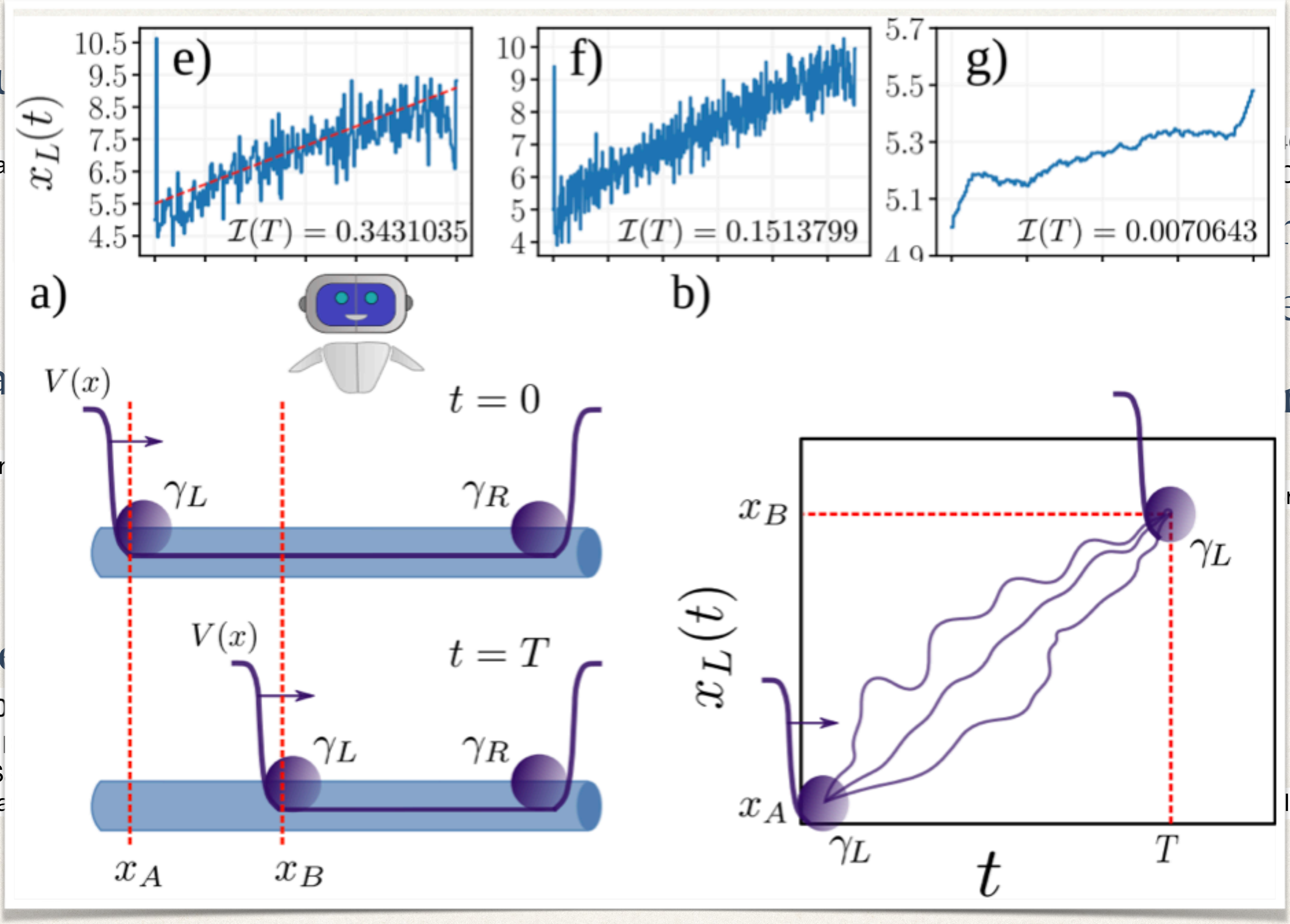

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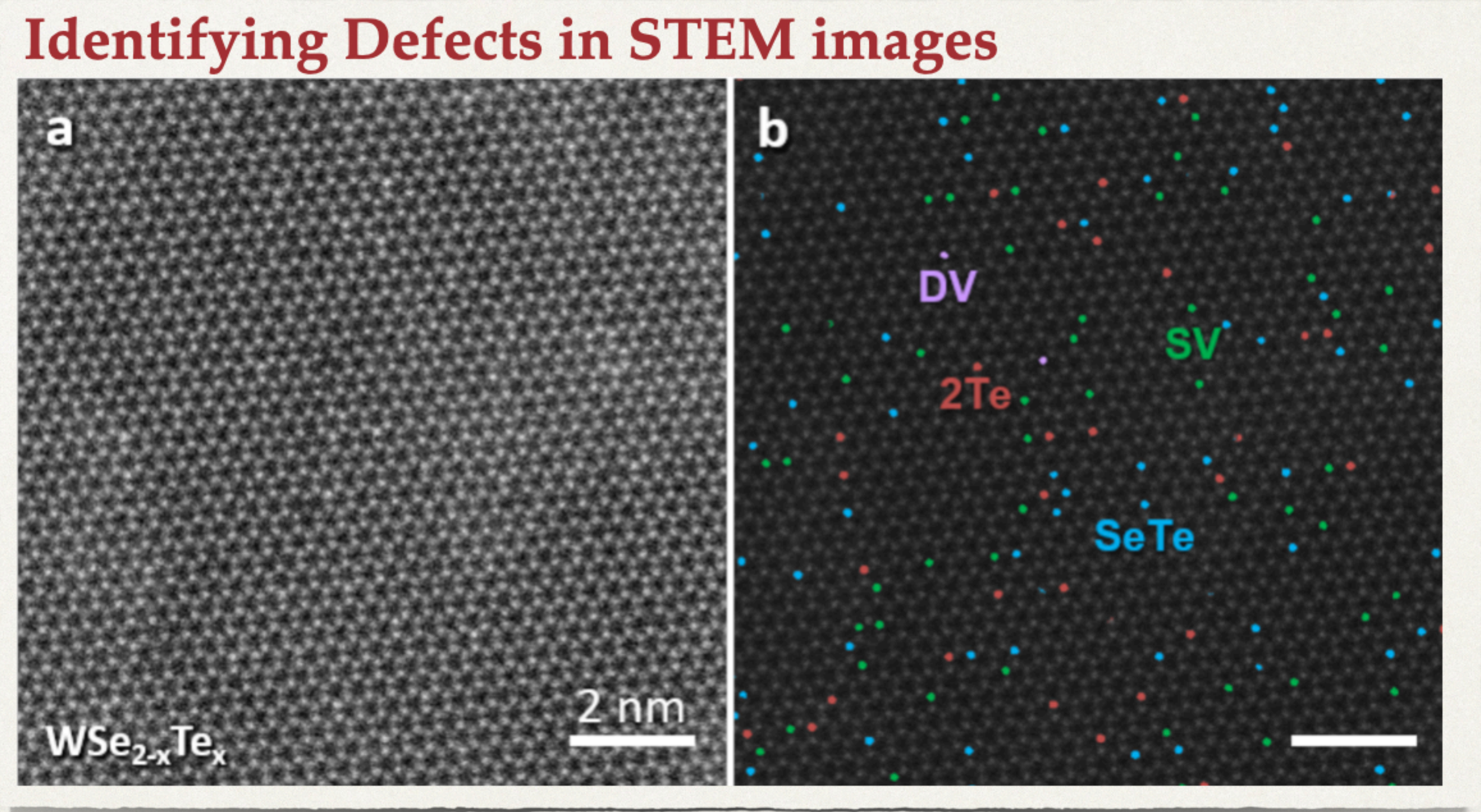

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Quantum Ground States

The electrons in materials are effectively at zero temperature.

To compute their properties, we need to compute the ground state of the physical system.

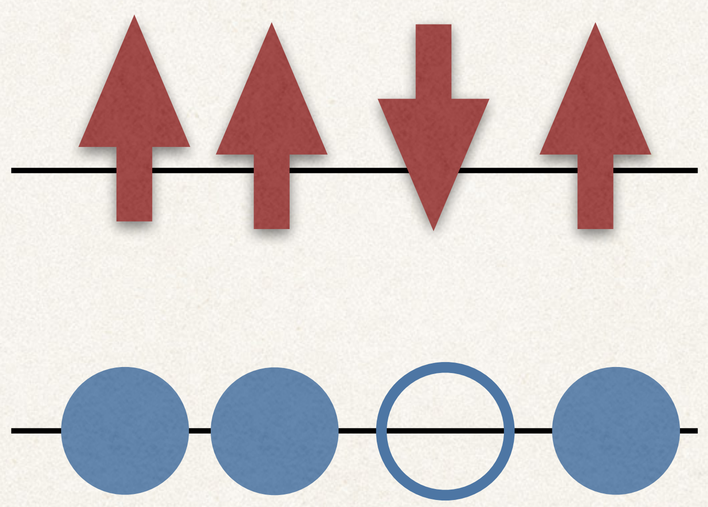
Quantum Ground States

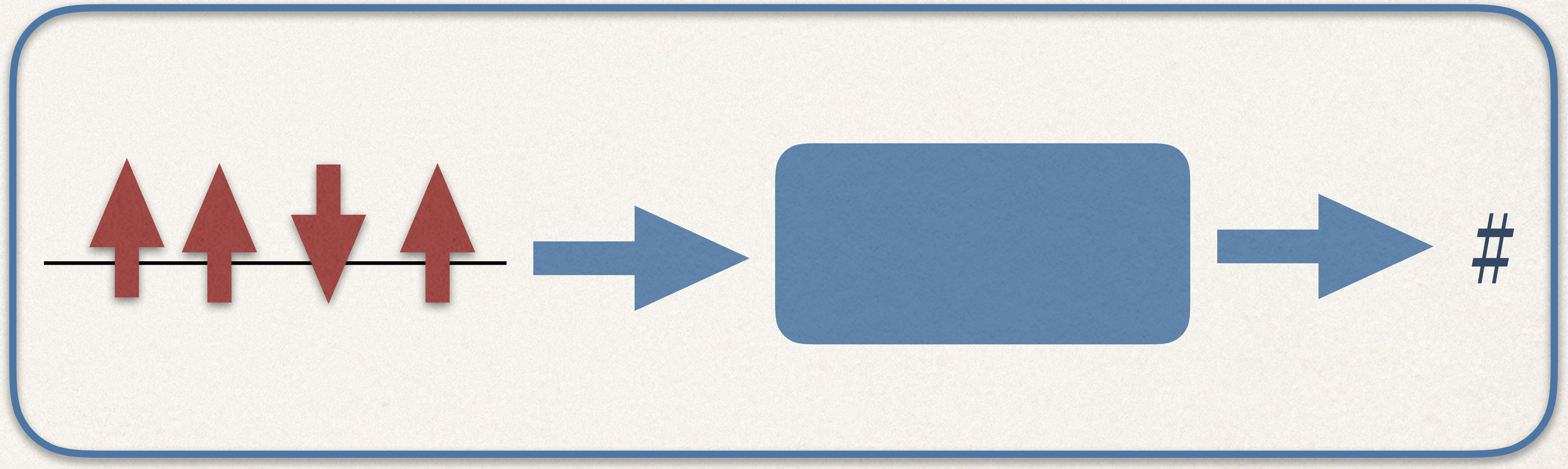
Solve for the ground state (lowest eigenvector) of $H\Psi = E\Psi$

H: a sparse $4^{200} \times 4^{200}$ matrix

Ψ: a 4^{200} vector ← Storing a quantum state requires more bits than there are atoms in the universe.

One approach is to compress Ψ.
Can think of $\Psi : \{1,1,0,1\} \to \mathbb{C}$





Variational Monte Carlo

Need a manifold of wave-functions $\Psi(\overrightarrow{p})$ specified by a set of parameters $\overrightarrow{p}$.

Evaluate $E(\overrightarrow{p}) = \sum_c |\Psi(c; \overrightarrow{p})|^2 E_L(c)$

Sample c from $|\Psi(c; \overrightarrow{p})|^2$ by Markov chain Monte Carlo.

Average $E_L(c)$ to get energy.

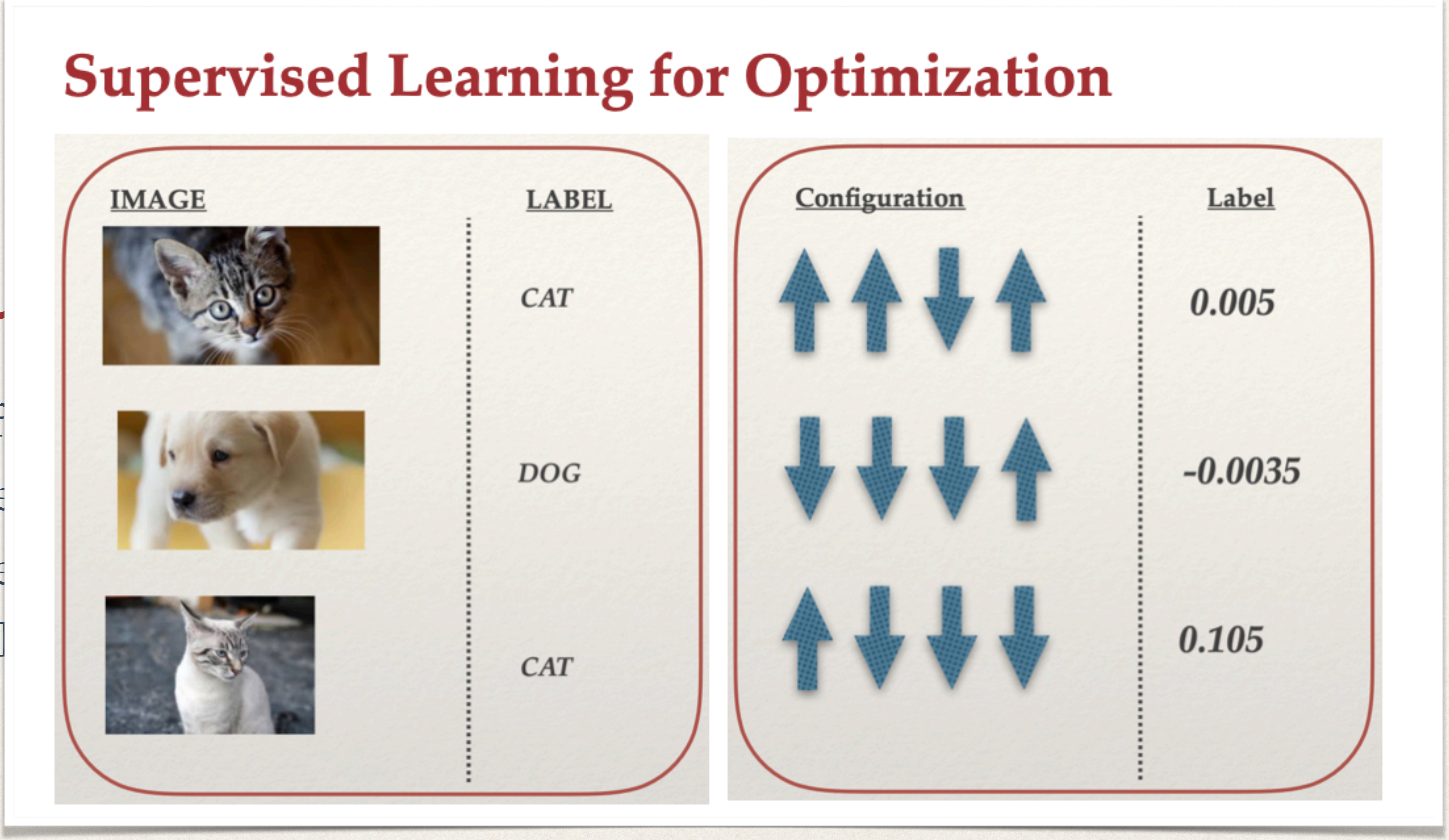
Average $\partial E_L(c)/\partial p$ (plus other terms) to get energy gradient $\partial E/\partial p$.

Step downhill in energy for parameters…

Variational Monte Carlo

Need a manifold of wave-functions $\Psi(\vec{p})$ specified by a set of parameters $\vec{p}$.

Evaluate $E(\vec{p}) =$



Sample c f

Average

Average

Step down

Wavefunction compression

Some Hamiltonians already have compressed forms…

$$H = \sum_{ij} c_i^\dagger c_j$$

⬅ Non-interacting fermions

Electrons only see each other through the Pauli-principle

Consider a 4-site 3-electron problem.

$$\left\{ \begin{matrix} \phi_1(r_1) & \phi_2(r_1) & \phi_3(r_1) \\ \phi_1(r_2) & \phi_2(r_2) & \phi_3(r_2) \\ \phi_1(r_3) & \phi_2(r_3) & \phi_3(r_3) \\ \phi_1(r_4) & \phi_2(r_4) & \phi_3(r_4) \end{matrix} \right.$$

Important property for any Fermion wave-function: swap electrons, sign changes…

Wavefunction compression

Some Hamiltonians already have compressed forms…

$$H = \sum_{ij} c_i^\dagger c_j$$

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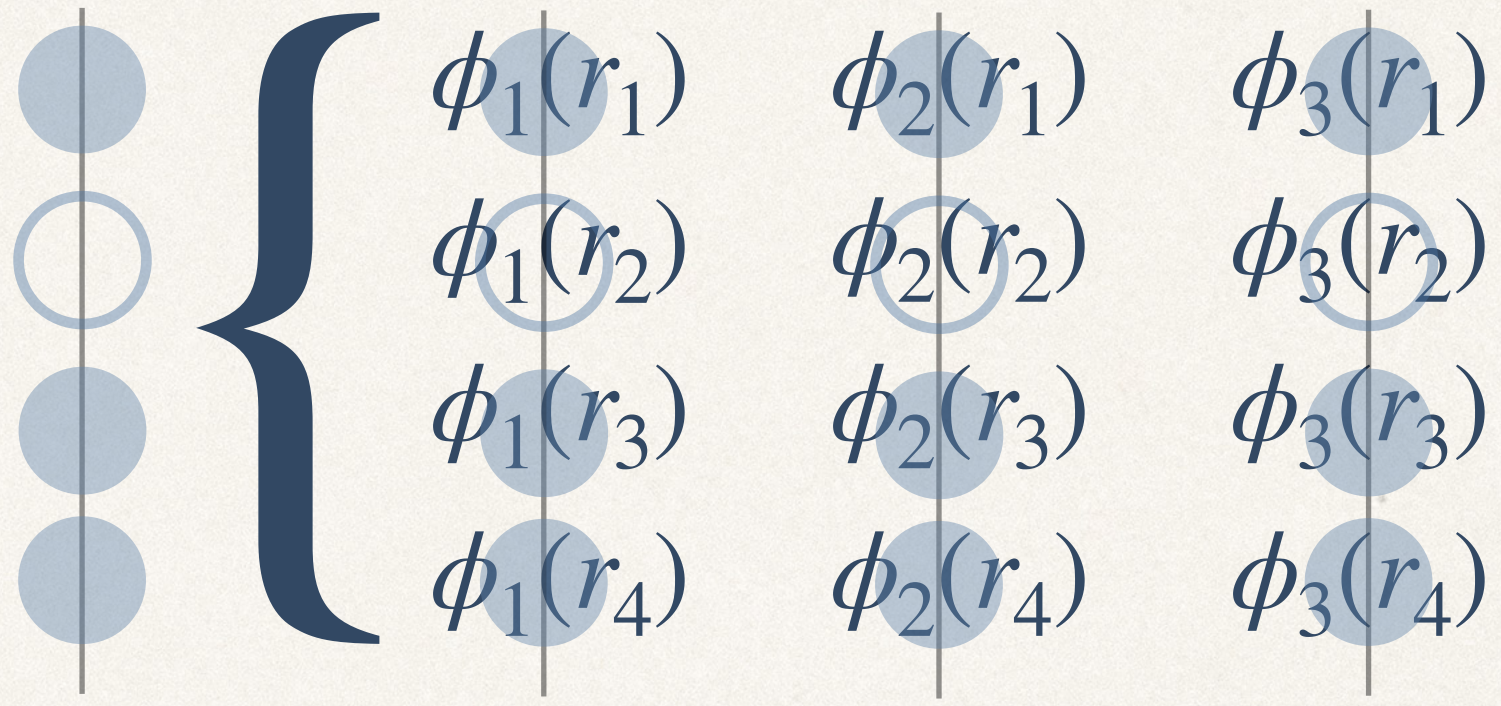

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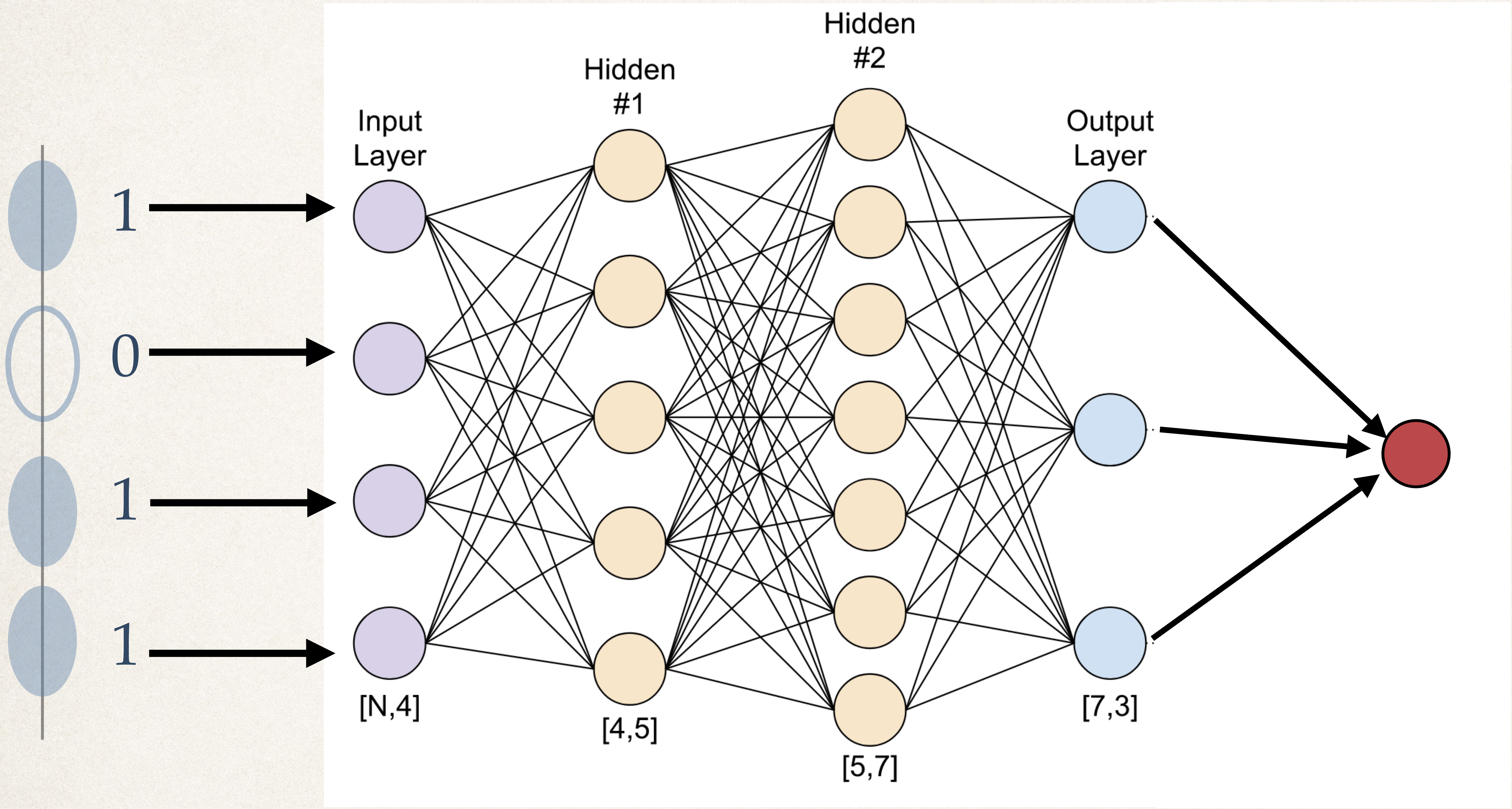


Usable Neural Architectures

FFNN

Unusable Neural Architectures

Transformers

Restricted Boltzmann Machines

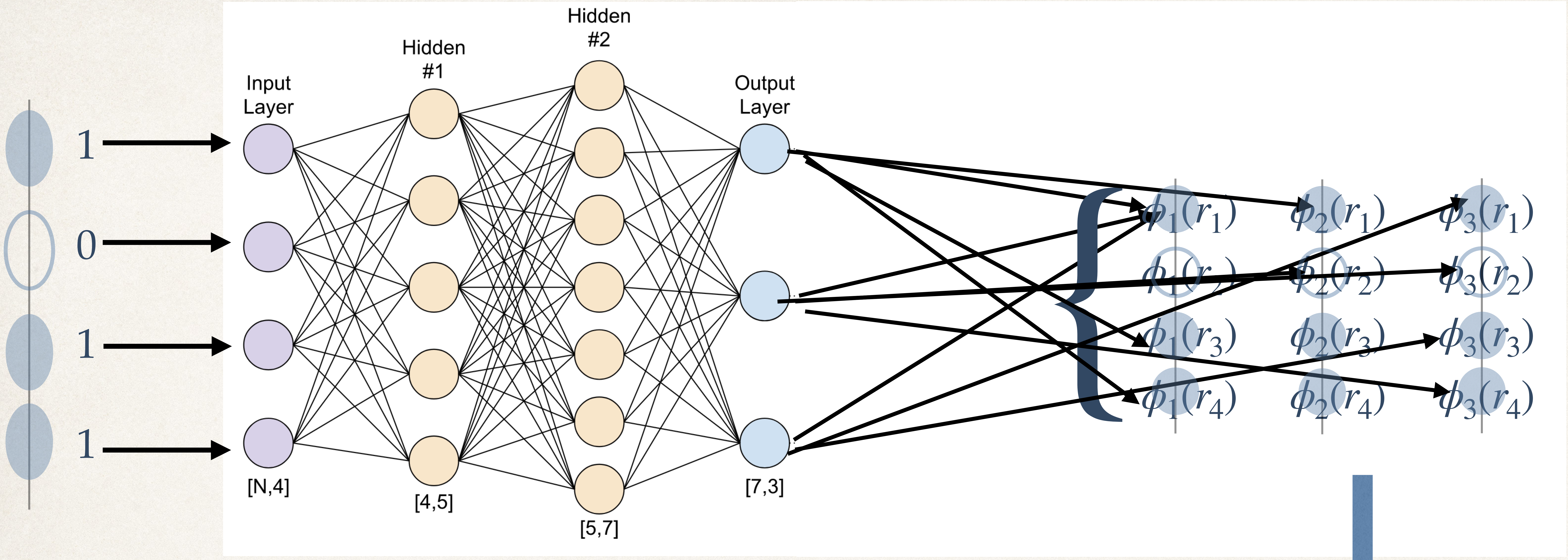
This has worked reasonably for `bosonic' wave-functions…

but appears impractical for electronic systems.

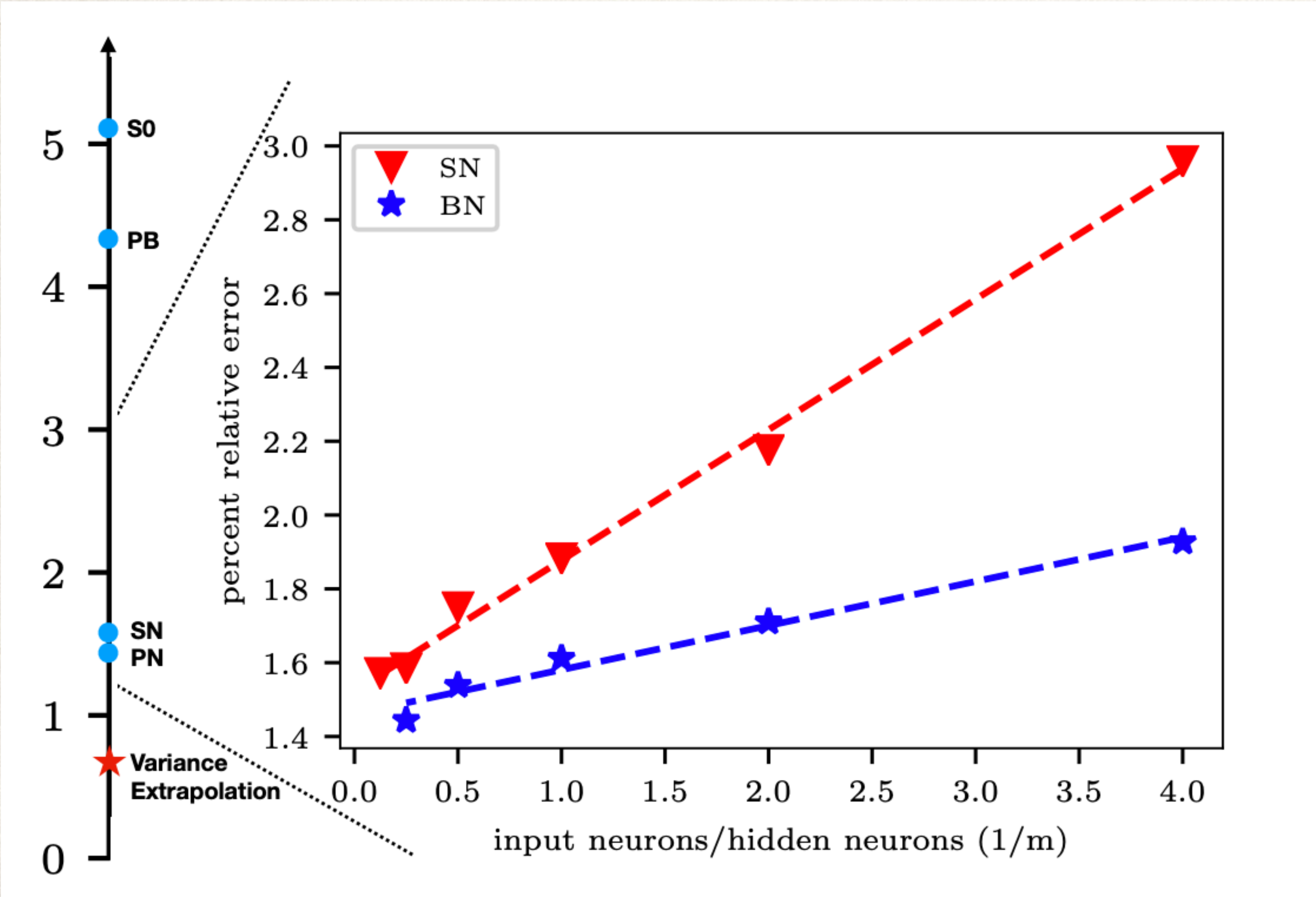
Not easy to get a determinant this way….

Neural Network Backflow

$O(N^4)$ per sweep

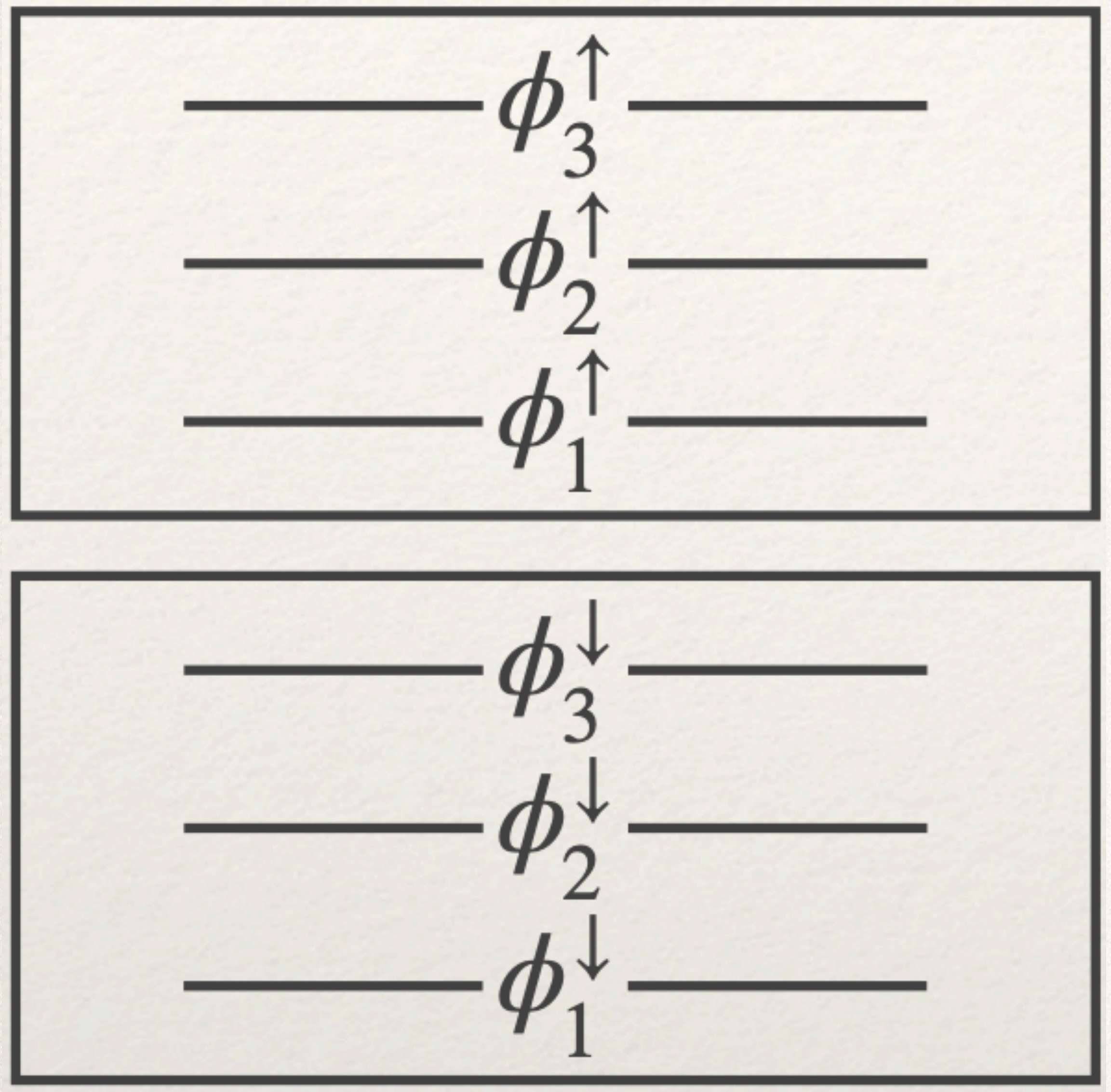


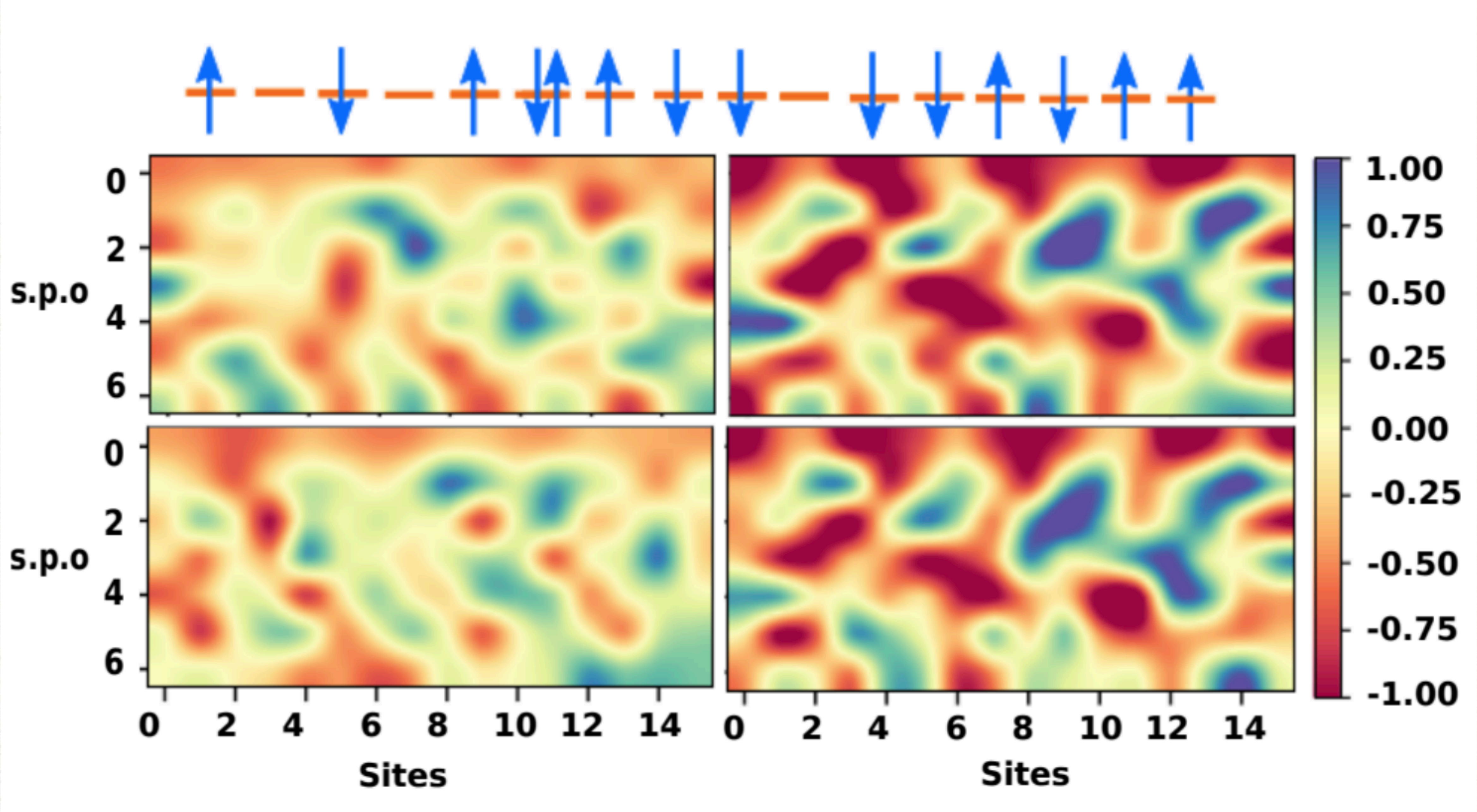
$$\det \begin{pmatrix} \phi_1(r_1) & \phi_2(r_1) & \phi_3(r_1) \\ \phi_1(r_3) & \phi_2(r_3) & \phi_3(r_3) \\ \phi_1(r_4) & \phi_2(r_4) & \phi_3(r_4) \end{pmatrix}$$



Configuration dependent single-particle orbitals

We not only get better energies; we restore the symmetry





Spin-up

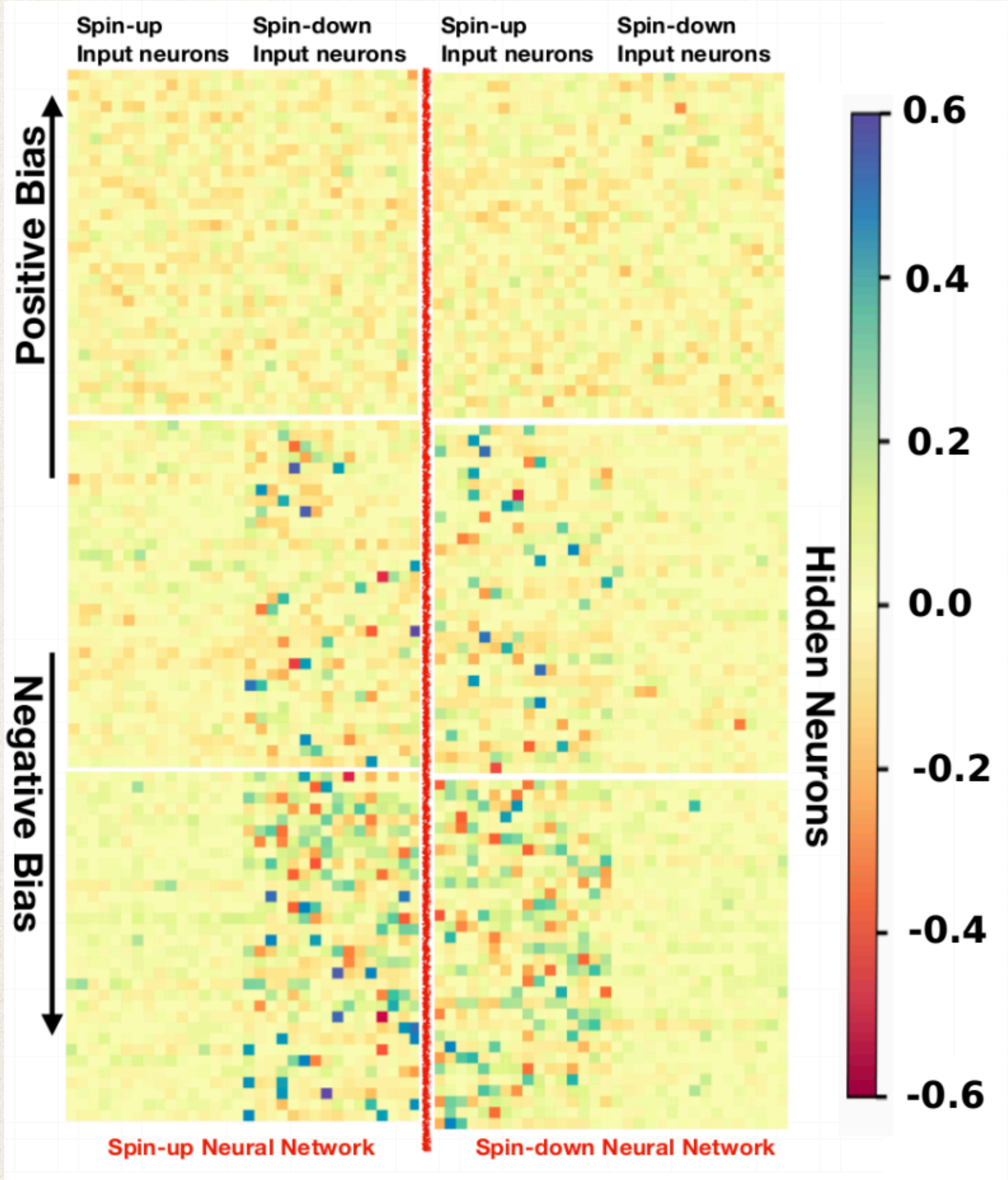
Spin-down

and change the signs…

$$\frac{\int |\Psi_{\mathrm{S0}}(x)|^2 \mathrm{sgn}(\Psi_{\mathrm{SN}}(x))\mathrm{sgn}(\Psi_{\mathrm{S0}}(x))dx}{\int |\Psi_{\mathrm{S0}}(x)|^2 dx} = 0.815$$

9% difference between signs

Opening the black box…



Quality and Time

Relative energy error	Slater-Jastrow	NNB	NNB neuron extrapolation	NNB variance extrapolation
4×4 Hubbard, n=0.75	$(3.6 \pm 6 \times 10^{-4})\%$	$(0.631 \pm 8 \times 10^{-4})\%$	0.607%	0.233%
4×4 Hubbard, n=0.875	$(5.4 \pm 2 \times 10^{-3})\%$	$(1.156 \pm 2 \times 10^{-3})\%$	1.152%	1.101%
4×4 Hubbard, n=1.0	$(5.9 \pm 2 \times 10^{-3})\%$	$(2.714 \pm 5 \times 10^{-3})\%$	2.700%	1.745%
16×4 Hubbard, n=0.875	$(5.9 \pm 2 \times 10^{-3})\%$	$(2.734 \pm 8 \times 10^{-3})\%$	2.592%	0.209%
12×8 Hubbard, n=0.875	$(6.3 \pm 3 \times 10^{-3})\%$	$(3.94 \pm 10^{-2})\%$	3.727%	0.655%
$4 \times 4 \times 3$ Kagome	$(1.8 \pm 10^{-5})\%$	$(1.093 \pm 4 \times 10^{-3})\%$	1.055%	0.286%

Time: $O(N^4)$

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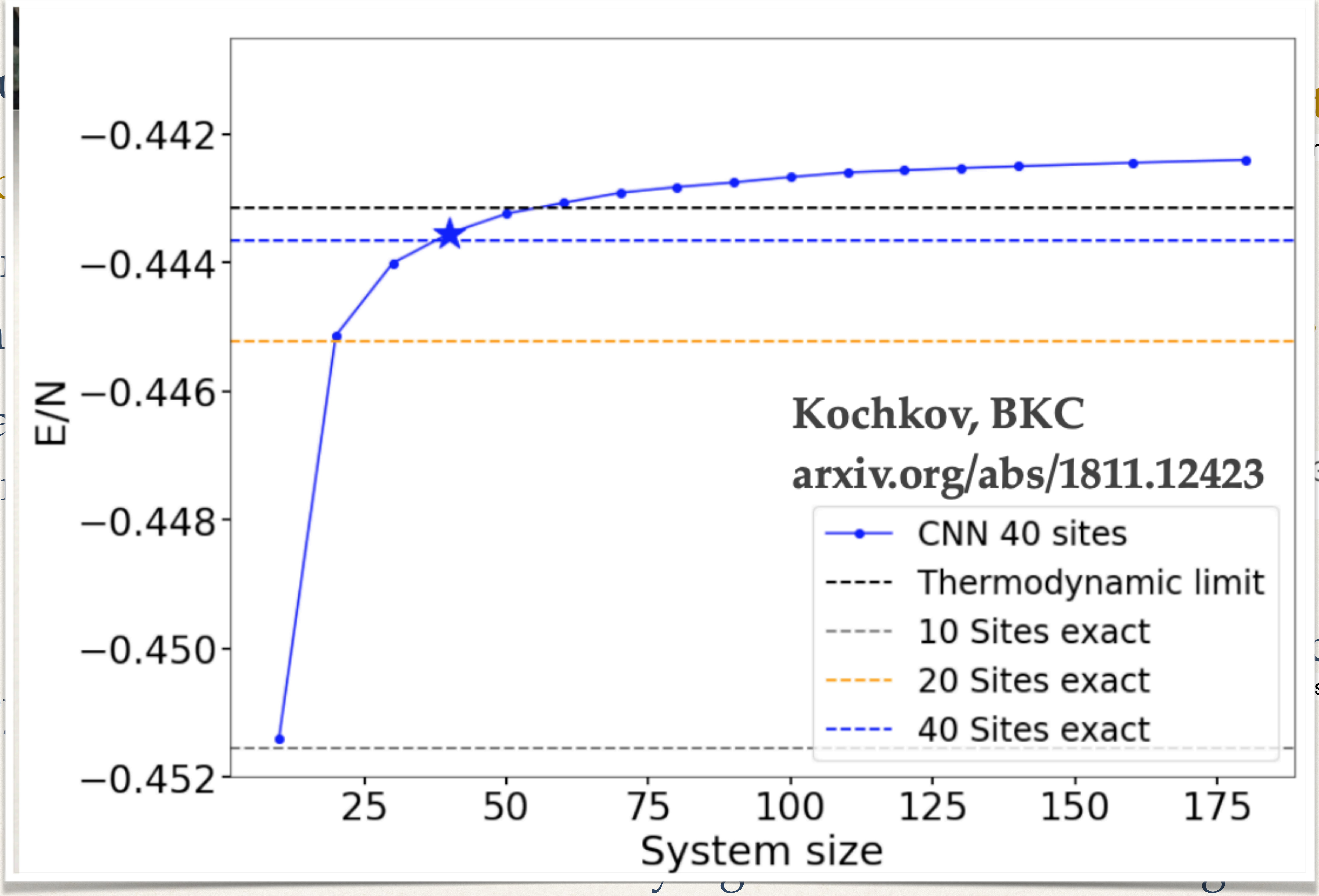

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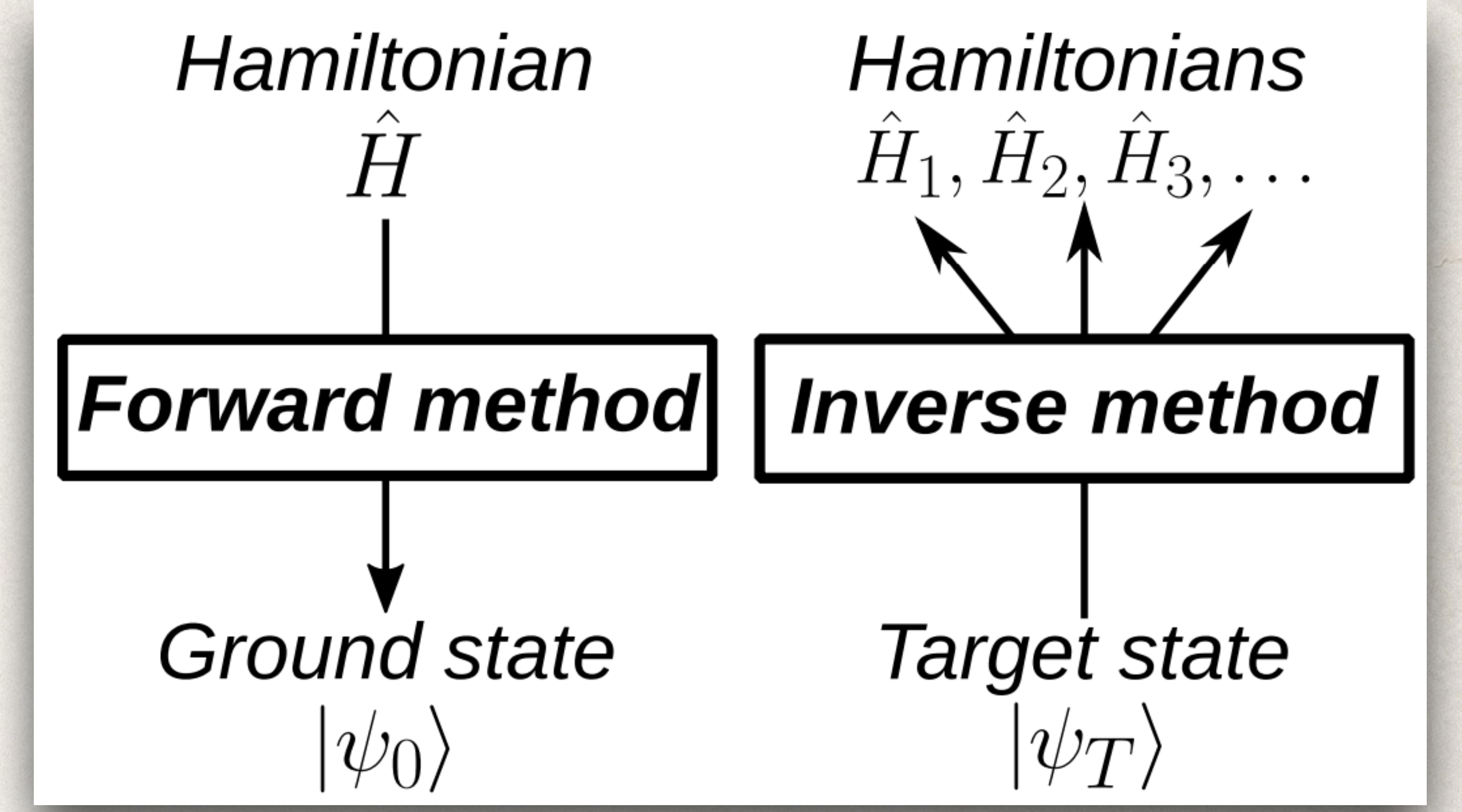
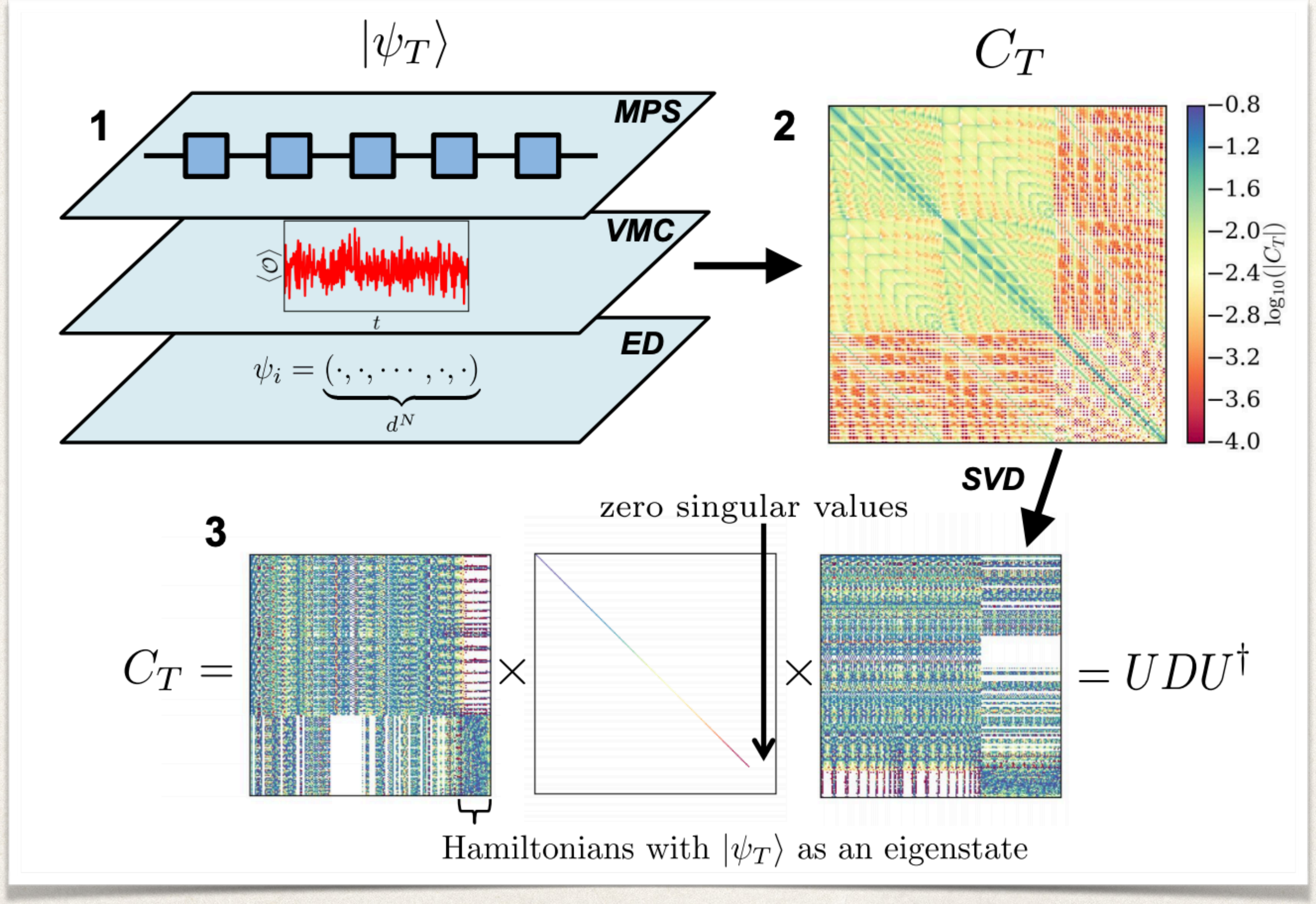
Inverse Methods…



The typical approach to condensed matter: $H \rightarrow \Psi$

An inverse approach: $\Psi \rightarrow H$

Quantum covariance matrix: $(C_T)_{ab} = \langle \Psi | h_a h_b | \Psi \rangle - \langle \Psi | h_a | \Psi \rangle \langle \Psi | h_b | \Psi \rangle$



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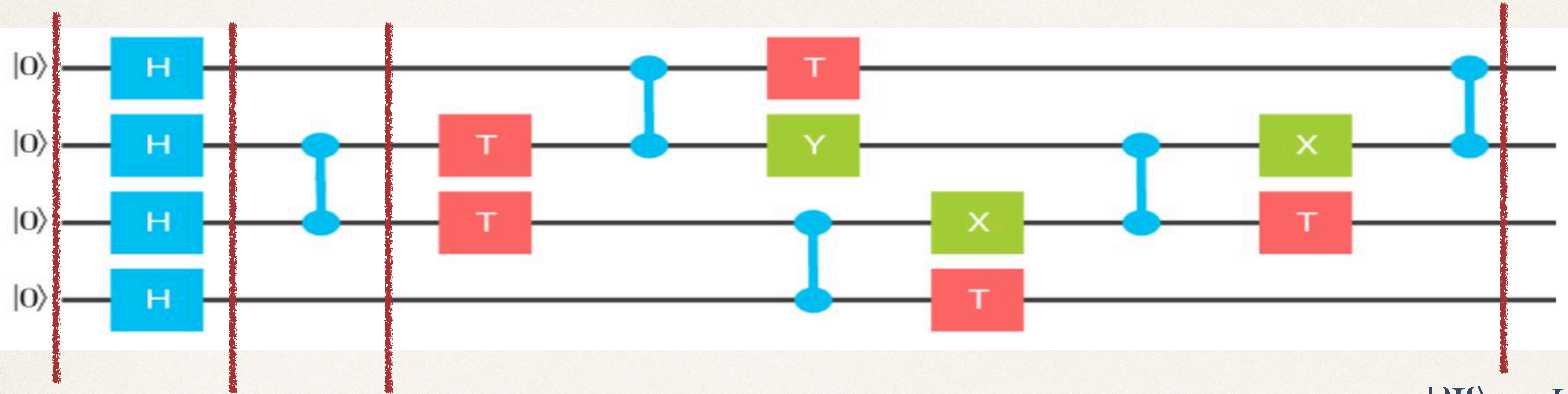
Simulating Quantum Circuits

State size: 2^n



$|0\rangle$ $U_1|0\rangle$ $U_2U_1|0\rangle$ $|\Psi\rangle \equiv U_9U_8\ldots U_2U_1|0\rangle$

Observables: $\langle\Psi|\hat{O}|\Psi\rangle$

Naive approach: Store $|\Psi\rangle$ and update exponentially large vector after each gate application.

Less naive approach: Tensor Networks; breaks down in two-dimensions.

Simulating Quantum Circuits

A new approach:

Quantum State → Probability Distribution → Compact with an Autoregressive Model

Quantum Gate → Quasi-stochastic matrix

Circuit → Update autoregressive model after each gate

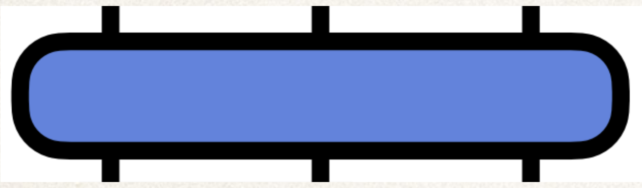
Simulating Quantum Circuits

A new approach:

Quantum State → Probability Distribution → Compact with an Autoregressive Model

$|\Psi\rangle \longrightarrow P(a_1, a_2, \ldots a_n) = Tr\left[(M^{a_1} \otimes M^{a_2} \otimes \ldots \otimes M^{a_n})\,|\Psi\rangle\langle\Psi|\right]$

Example for $n = 3$



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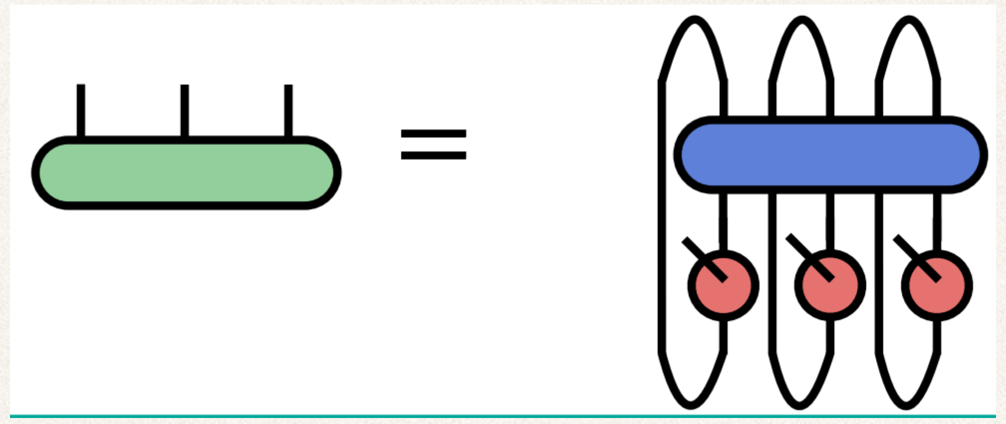
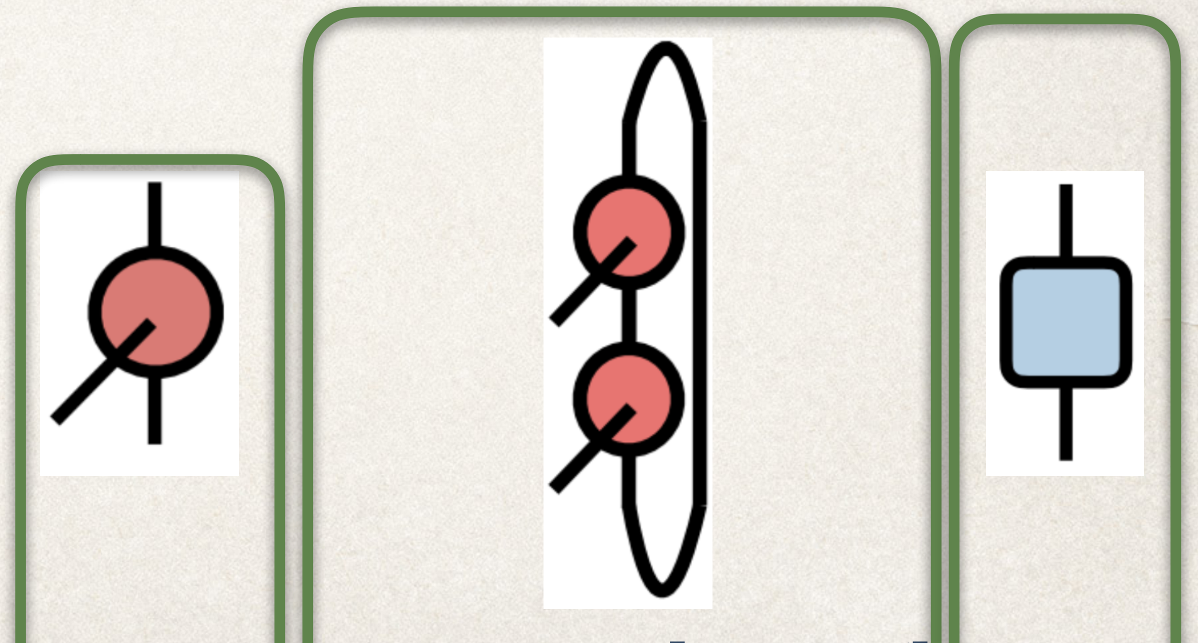


Projector Operator Value Measurements (POVM)



M^{a_i} $\quad T_{a_i,a_i'} = Tr\left[M^{a_i} M^{a_i'}\right]$ $\quad T^{-1}_{a_i,a_i'}$

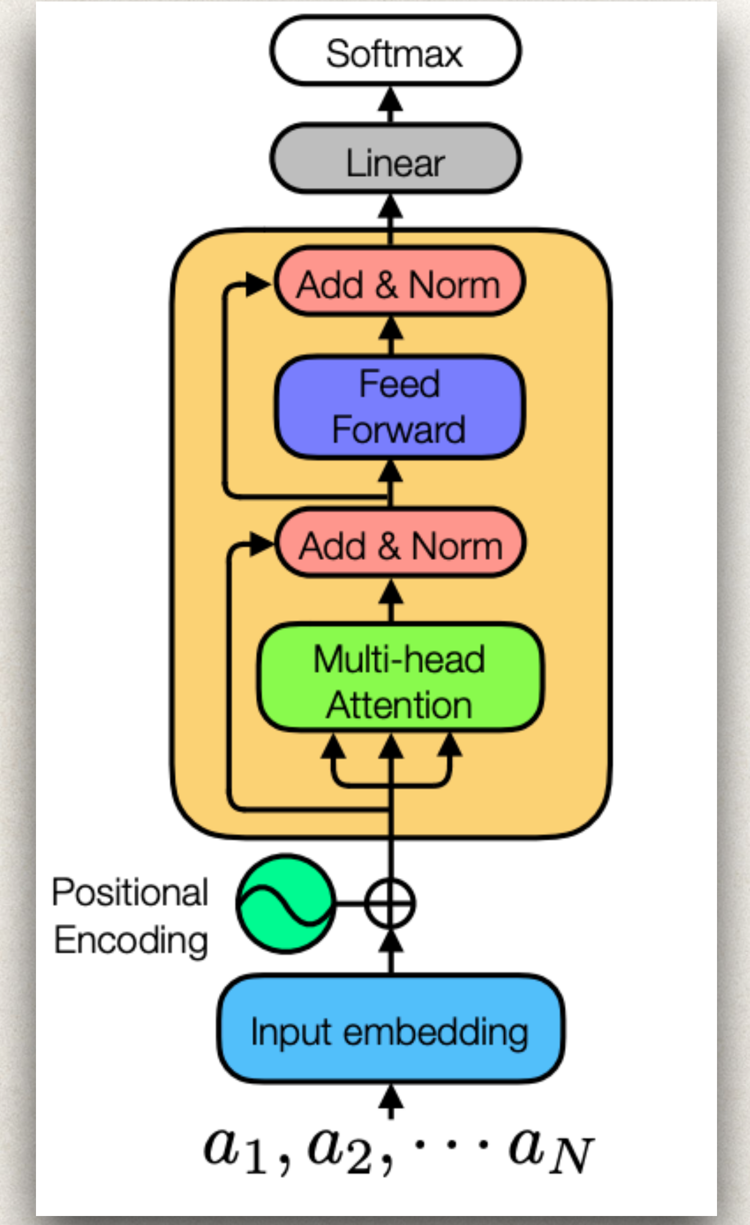
Simulating Quantum Circuits

A new approach:

Quantum State → Probability Distribution → Compact with an Autoregressive Model

$$P(a_1, a_2, \ldots a_n) = Tr\left[(M^{a_1} \otimes M^{a_2} \otimes \ldots \otimes M^{a_n})\,|\Psi\rangle\langle\Psi|\right]$$

Transformer



$$p_\theta(\boldsymbol{a}) = \prod_k p_\theta(a_k | a_1, a_2, \cdots, a_{k-1})$$

Autoregressive models: sequentially generate $a_i \in \{1,2,3,4\}$

Can sample without Markov chain Monte Carlo; no autocorrelation time.

Can compute amplitude (with normalization…)

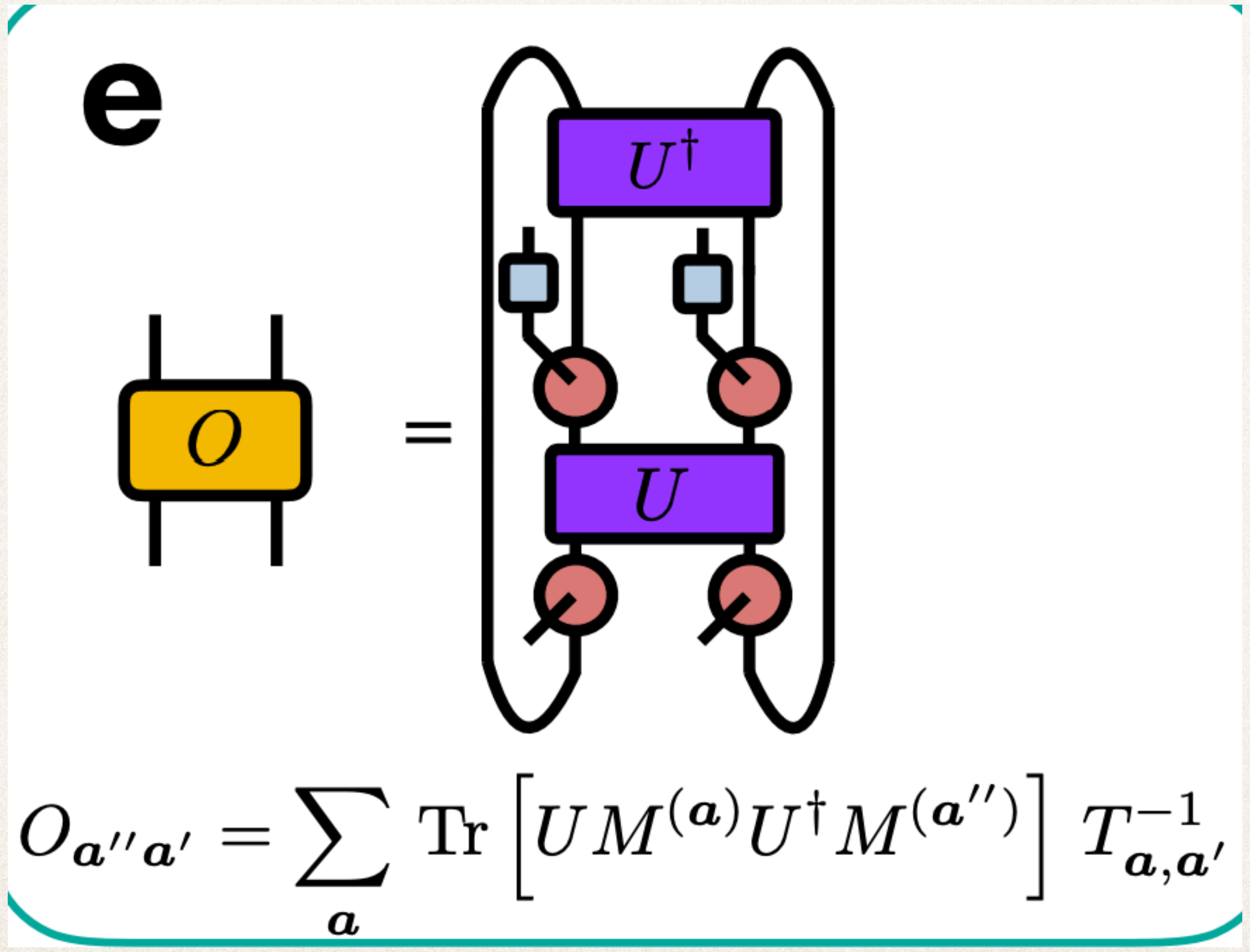
Simulating Quantum Circuits

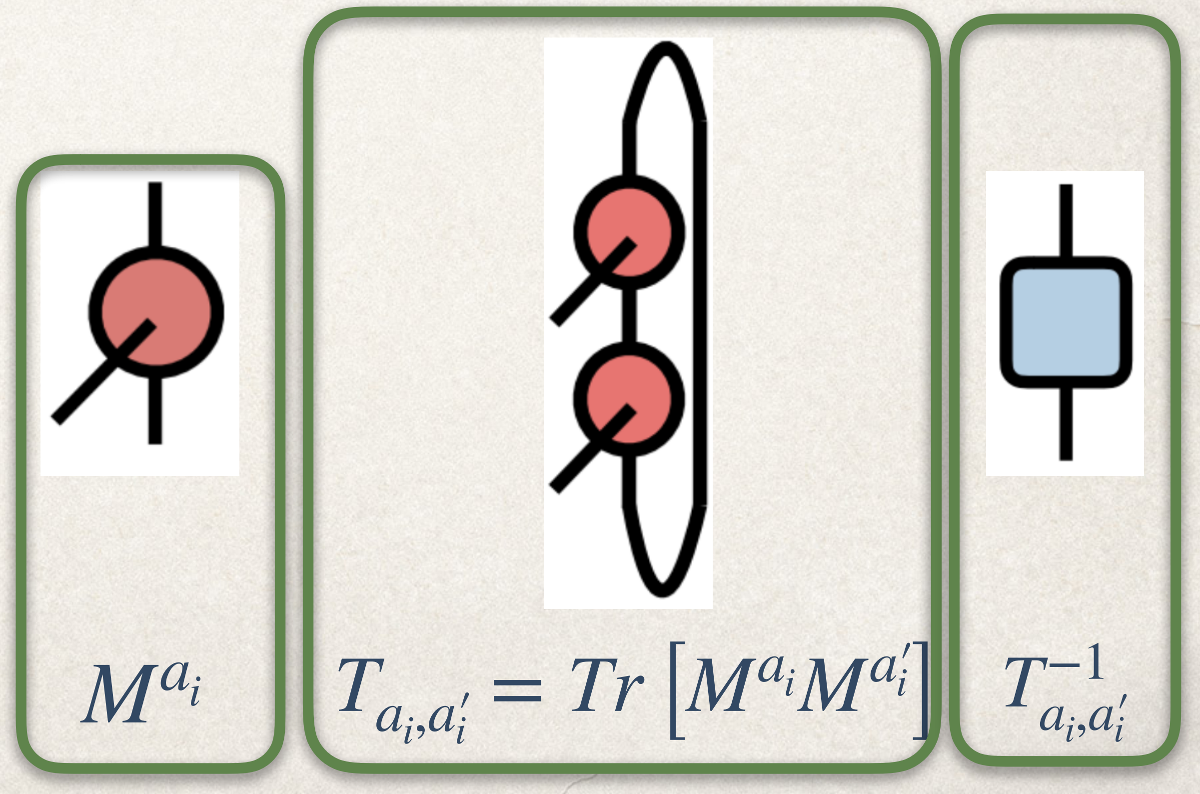
A new approach:

Quantum Gate → Quasi-stochastic matrix

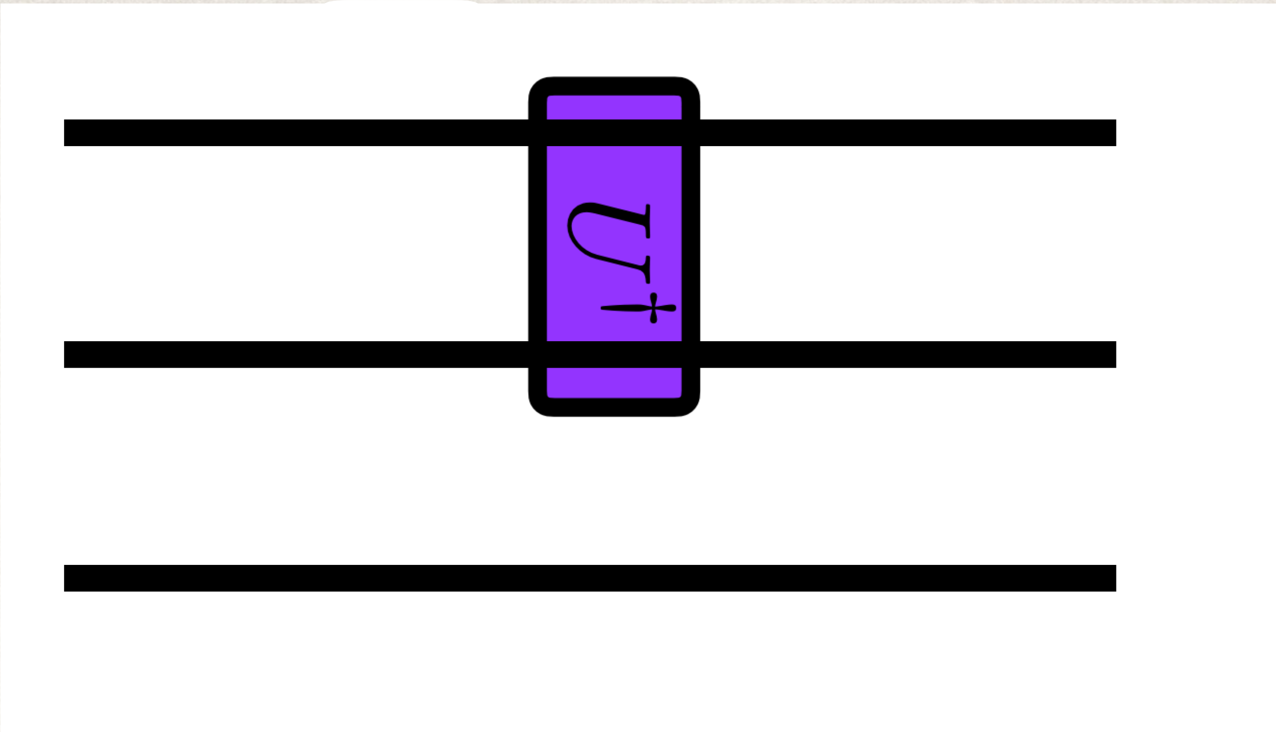
U: 2 qubit unitary

$$O_{\mathbf{a},\mathbf{a}'} = \sum_{\mathbf{a}} Tr\left[UM^{(\mathbf{a})}U^{\dagger}M^{(\mathbf{a}'')}\right] T^{-1}_{\mathbf{a},\mathbf{a}'}$$





$|\Psi\rangle$



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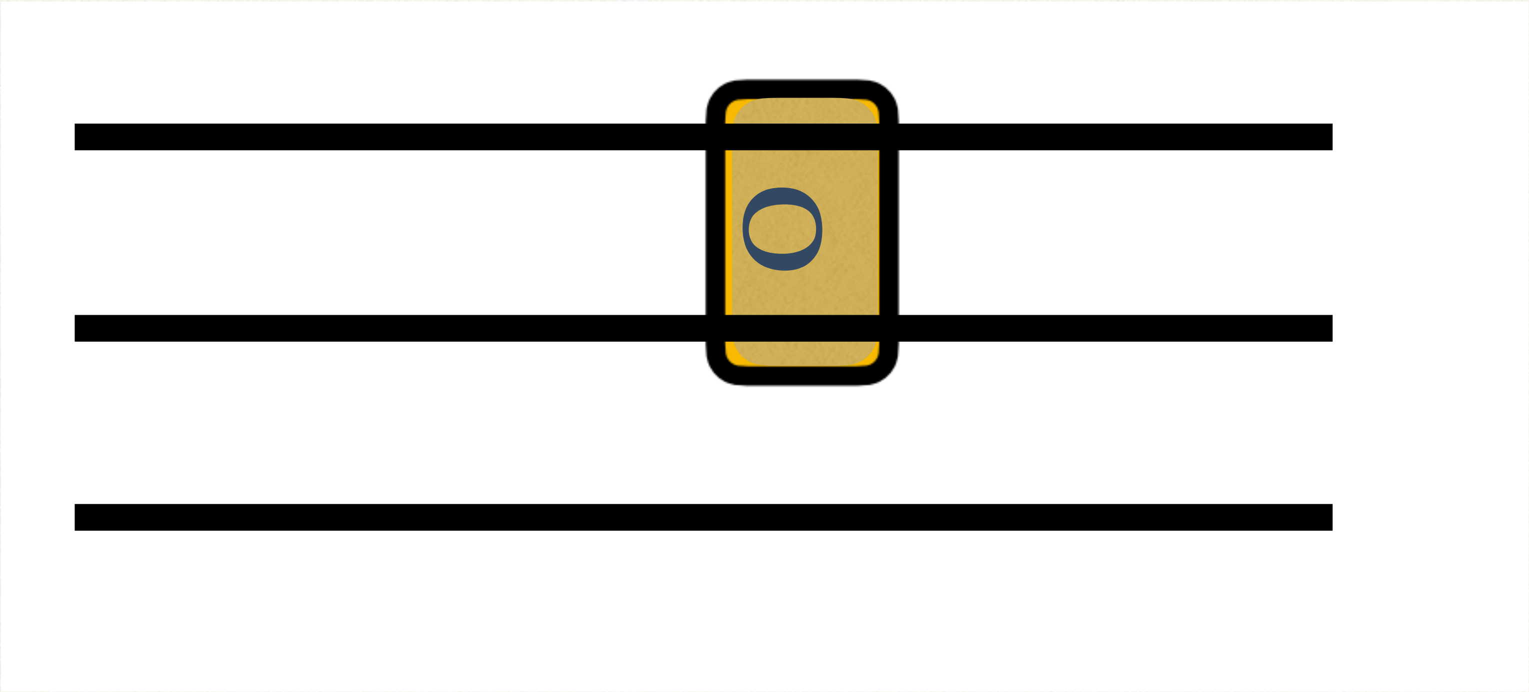


$$\mathrm{KL}(P^{(e)}_{i+1}\,||\,P_{\theta_{i+1}}) = -\sum_a P^{(e)}_{i+1}(a)\log\left(\frac{P_{\theta_{i+1}}(a)}{P^{(e)}_{i+1}(a)}\right)$$

$$\nabla_{\theta_{i+1}} KL(P^{(e)}_{i+1}\,||\,P_{\theta_{i+1}})$$

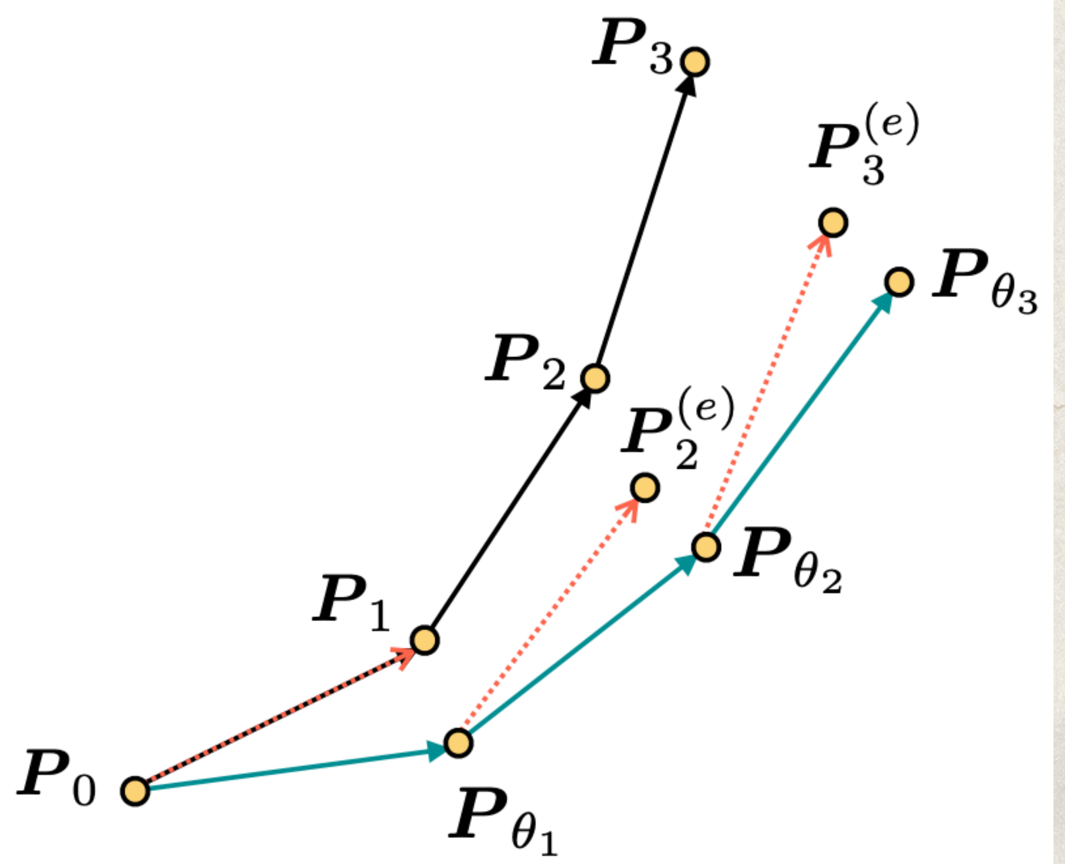
$$= -E_{a\sim P_{\theta_{i+1}}(a)}\left[\left(\frac{P^{(e)}_{i+1}(a)}{P_{\theta_{i+1}}(a)} - k\right)\nabla_{\theta_{i+1}}\log(P_{\theta_{i+1}}(a))\right]$$

$$k = -E_{a\sim P_{\theta_{i+1}}(a)}\left[\left(\frac{P^{(e)}_{i+1}(a)}{P_{\theta_{i+1}}(a)}\right)\right]$$

$$P^{(e)}_{i+1} = \sum_{a'} O^{(i+1)}_{a,a'} P_{\theta_i}(a')$$

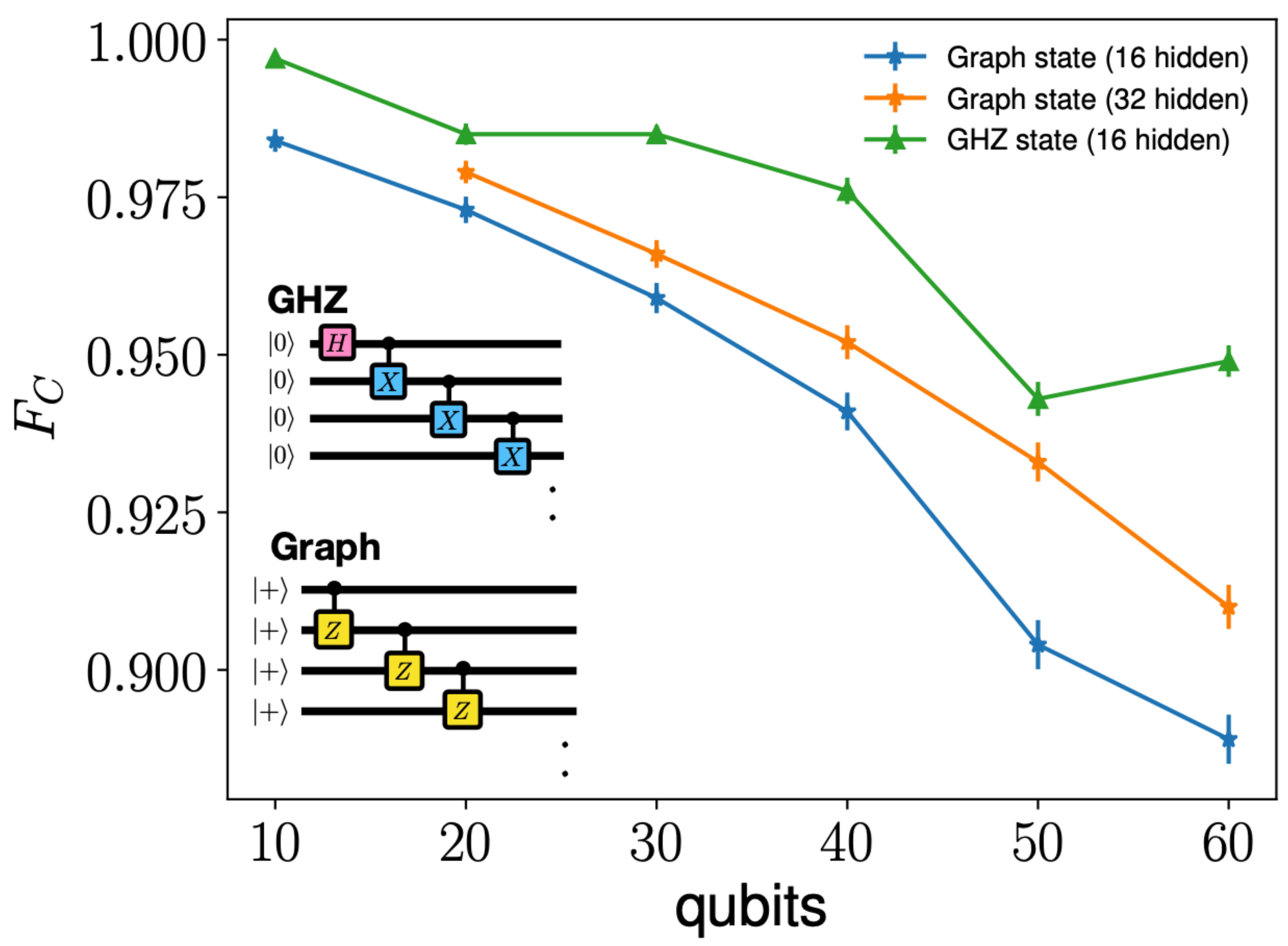
Algorithm: To sample k and $\nabla_{\theta_{i+1}} KL(P^{(e)}_{i+1}\,||\,P_{\theta_{i+1}})$

1. Sample a from $P_{\theta_{i+1}(a)}$
2. Ask transformer for $P_{\theta_{i+1}(a)}$
3. Evaluate $P^{(e)}_{i+1}(a)$ explicitly
4. Automatic differentiation for $\nabla_{\theta_{i+1}}\log(P_{\theta_{i+1}}(a))$

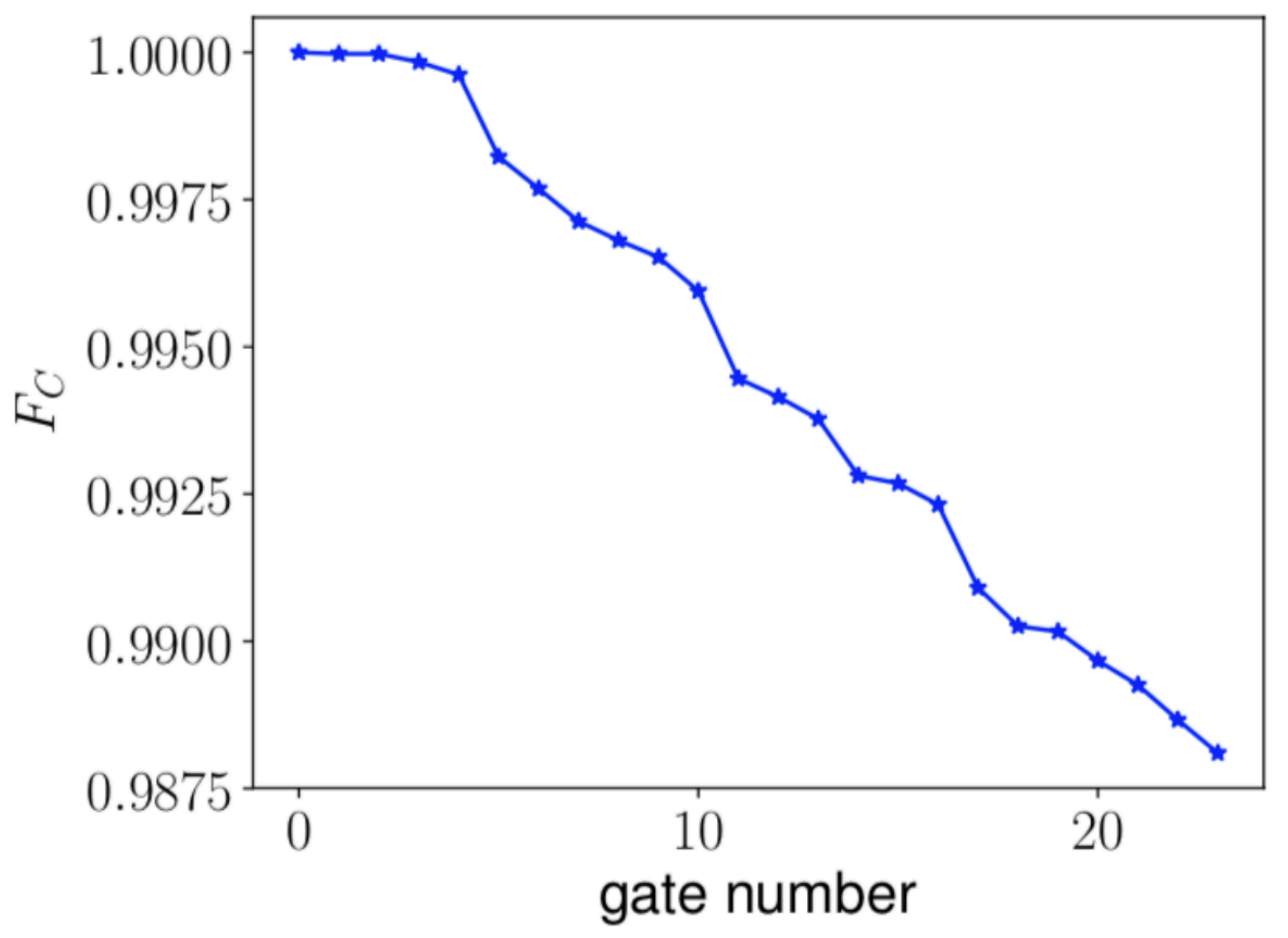


How do we do?

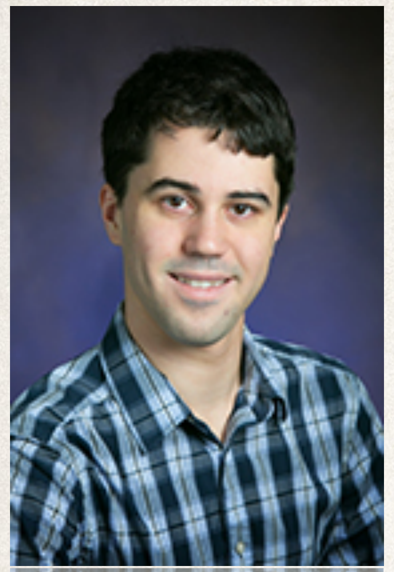
$$F_c(p_a, p_b) = \sum_a \sqrt{p_a p_b}$$



VQE (6 qubits)



Eli



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Machine Learning Quantum Matter and Quantum Computing

Majoranas in superconductors

arXiv:2008.09128

Luuk Coopmans, Di Luo, Graham Kells, Bryan K. Clark, Juan Carrasquilla

Quantum Dynamics

arXiv:2009.05580

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Quantum Ground States

Sign-structures

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Deep Learning with Symmetries

Wave-functions for Infinite Systems

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Optimizing wave-functions from supervised learning

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